

Supplementary Information for

**Surface decoration of phosphorene nanoribbons via 4d transition
metal atoms for spintronics**

Xiao-Xiao Fu^{a*}, Yue Niu^a, Ze-Wen Hao, Mi-Mi Dong, Chuan-Kui Wang^{*}

Shandong Key Laboratory of Medical Physics and Image Processing & Shandong Provincial
Engineering and Technical Center of Light Manipulations, School of Physics and Electronics,
Shandong Normal University, Jinan 250358, China

^a These authors contributed equally to this work.

^{*} E-mail: fuxiaoxiao@sdu.edu.cn; ckwang@sdu.edu.cn

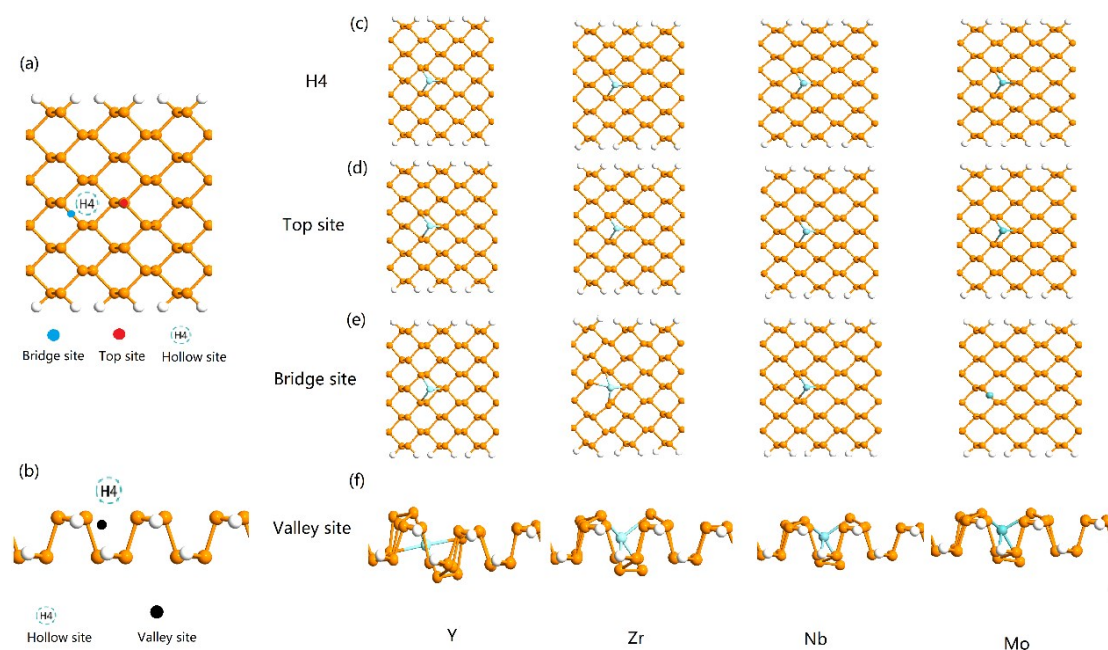


Fig. S1 (a-b) Schematic views and (c-f) relaxed structures of X-adsorbed hydrogenated armchair phosphorene nanoribbons ($X = Y, Zr, Nb$ and Mo) with hollow, top, bridge and valley sites.

Table S1 The formation energy (E_f) and magnetic moment (M) of the X-adsorbed ($X = Y, Zr, Nb$ and Mo) phosphorene nanoribbons with different initial adsorption sites.

Atoms	Adsorption Site	E_f (eV)	M
Y	Hollow site	-3.85	0.70
	Top site	-3.86	0.72
	Bridge site	-3.86	0.72
	Valley site	-5.29	0.00
Zr	Hollow site	-4.62	1.58
	Top site	-4.62	1.59
	Bridge site	-4.42	1.52
	Valley site	-6.24	0.00
Nb	Hollow site	-4.29	0.95
	Top site	-4.29	0.94
	Bridge site	-4.29	0.94
	Valley site	-6.04	0.00
Mo	Hollow site	-2.55	3.45
	Top site	-2.55	3.45
	Bridge site	-1.52	5.19
	Valley site	-4.37	0.00

Table S2. Parameters for the adsorption with different hollow sites (H1-H4) and the substitutional doping (S) of 4d transition metal atoms ($X = Y, Zr, Nb$ and Mo) on hydrogenated armchair phosphorene nanoribbons, including the distortion of nanoribbons (ΔY_{\max} , the maximal displacement in the Y direction of P atoms from their initial position), the minimum X-P distance (d_{X-P}), the formation energy (E_f) and the magnetic moment (M).

Atoms	Site	ΔY_{\max} (Å)	d_{X-P} (Å)	E_f (eV)	M
Y	H1	0.338	2.68	-3.94	0.72
	H2	0.106	2.70	-3.84	0.75
	H3	0.143	2.72	-3.84	0.71
	H4	0.150	2.72	-3.85	0.70
	S	0.468	2.69	-5.93	0.00
Zr	H1	0.400	2.53	-4.68	1.48
	H2	0.122	2.55	-4.58	1.60
	H3	0.130	2.55	-4.61	1.59
	H4	0.137	2.55	-4.62	1.58
	S	0.573	2.58	-6.84	0.63
Nb	H1	0.436	2.39	-4.40	0.94
	H2	0.138	2.36	-4.25	0.95
	H3	0.149	2.36	-4.28	0.94
	H4	0.149	2.36	-4.29	0.95
	S	0.567	2.44	-6.40	0.00
Mo	H1	0.0904	2.44	-2.40	3.59
	H2	0.0782	2.45	-2.51	3.50
	H3	0.0866	2.45	-2.54	3.47
	H4	0.0899	2.45	-2.55	3.45
	S	0.2783	2.48	-4.51	2.82

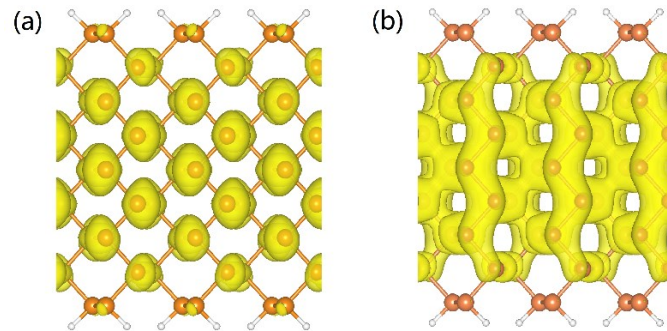


Fig. S2 Charge density of (a) VBM and (b) CBM of the pure phosphorene nanoribbon.

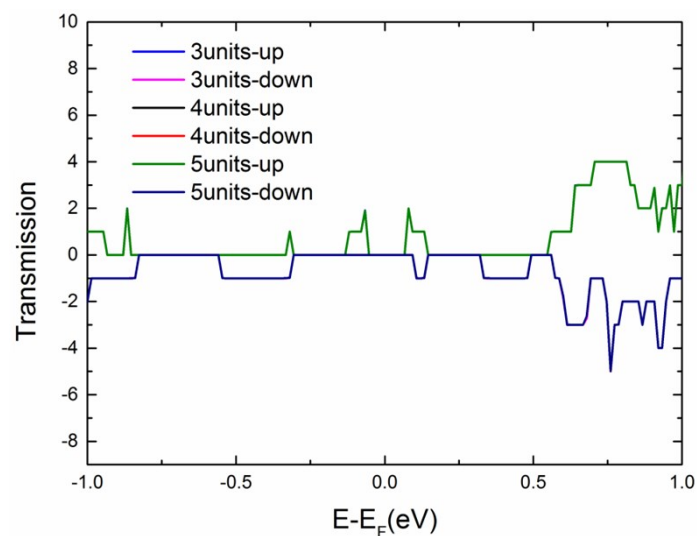


Fig. S3 Transmission spectra of the Mo-adsorbed phosphorene nanoribbons with central region containing 3-, 4- and 5-units for parallel spin configurations, respectively. The consistency of these transmission spectra indicates the convergence of the length of nanoribbons taken account in the transport calculation.

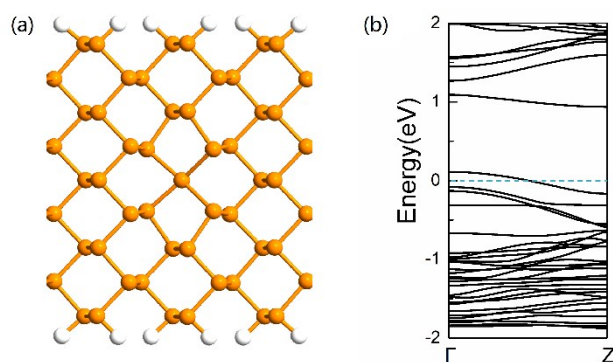


Fig. S4 (a) The relaxed geometric structure and (b) the band structure of the pristine phosphorene nanoribbon with the single-atom vacancy.

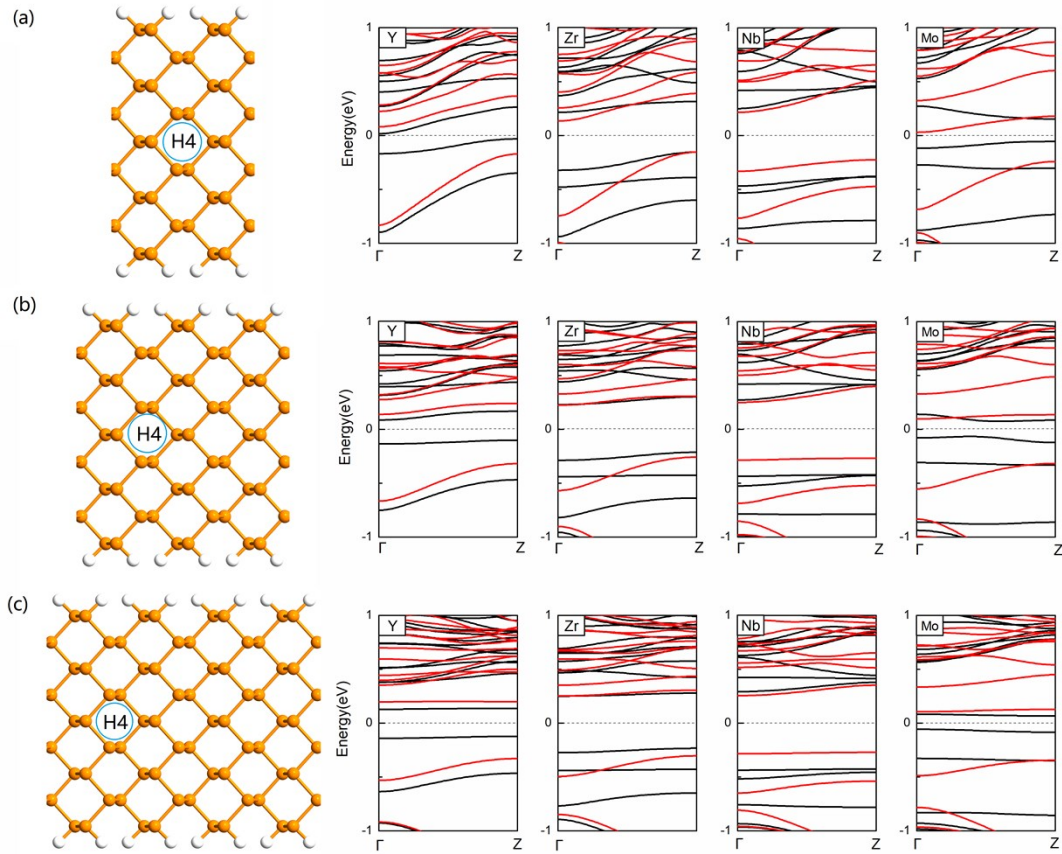


Fig. S5 (a)-(c) The schematic structure and the band structure of the X-adsorbed phosphorene nanoribbons (X=Y, Zr, Nb and Mo) with different concentrations.

Table S3 The band gap and magnetic moment (M) for the X-adsorbed phosphorene nanoribbons (X=Y, Zr, Nb and Mo) with the concentration of 1.1%, 1.5% and 2.2%.

Atoms	Concentration (%)	Band gap (eV)	M
Y	1.1	0.25	0.66
	1.5	0.19	0.70
	2.2	0.05	0.68
Zr	1.1	0.48	1.60
	1.5	0.43	1.58
	2.2	0.29	1.57
Nb	1.1	0.53	0.95
	1.5	0.52	0.95
	2.2	0.44	0.95
Mo	1.1	0.12	3.46
	1.5	0.13	3.45
	2.2	0.08	3.37

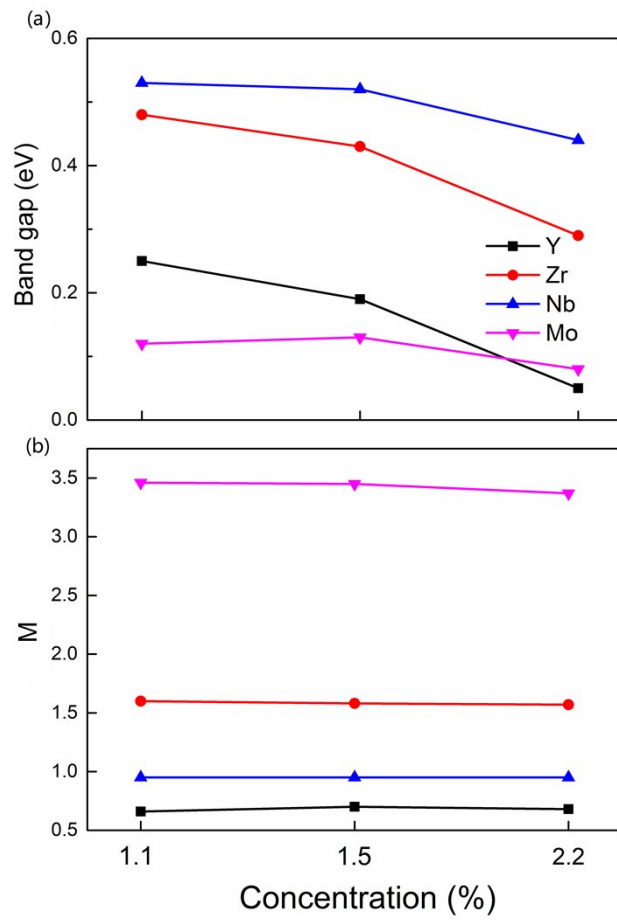


Fig. S6 (a) and (b) The variation of the band gap and magnetic moment of the X-adsorbed phosphorene nanoribbons (X=Y, Zr, Nb and Mo) with adsorption concentration (1.1%, 1.5% and 2.2%).